

PLS Mean Centering

This example shows how to compute Partial Least Squares (PLS) with mean centering.

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Supporting Information

A Practical Guide to Chemometric Analysis of Optical Spectroscopic Data

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Partial Least Squares (PLS) with Mean Centering

Partial least squares usually uses mean-centered data to compute C_{pls} using the weights from the SIMPLS algorithm with r latent variables.

```
X = A_train;
Y = C_train;

X0 = X - mean(X,1);
Y0 = Y - mean(Y,1);
[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r);

B_pls = Weights * Y_loadings';

C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
```

Partial Least Squares (PLS) without Mean Centering

The following is PLS without mean centering.

```
X = A_train;
Y = C_train;

[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X, Y, r);
```

```
B_pls = Weights * Y_loadings';
```

```
C_pls = A_unknown * B_pls;
```

Combined algorithm

To make it easier to run with the rest of the tools in the PNNL toolbox, we combined mean-centered and non-mean-centered into one function with meanCentered as an optional argument. When meanCentered is not used as an input, then the default is to compute without mean-centered data.

```
function [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, r, meanCentered)
    if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r); %#ok<ASGLU>

    B_pls = Weights * Y_loadings';

    if meanCentered
        C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
    else
        C_pls = A_unknown * B_pls;
    end
end
```

Napalm Data

Load the included napalm data to run the PLS algorithms.

```
clearvars
load pnnl_napalm_data
whos
```

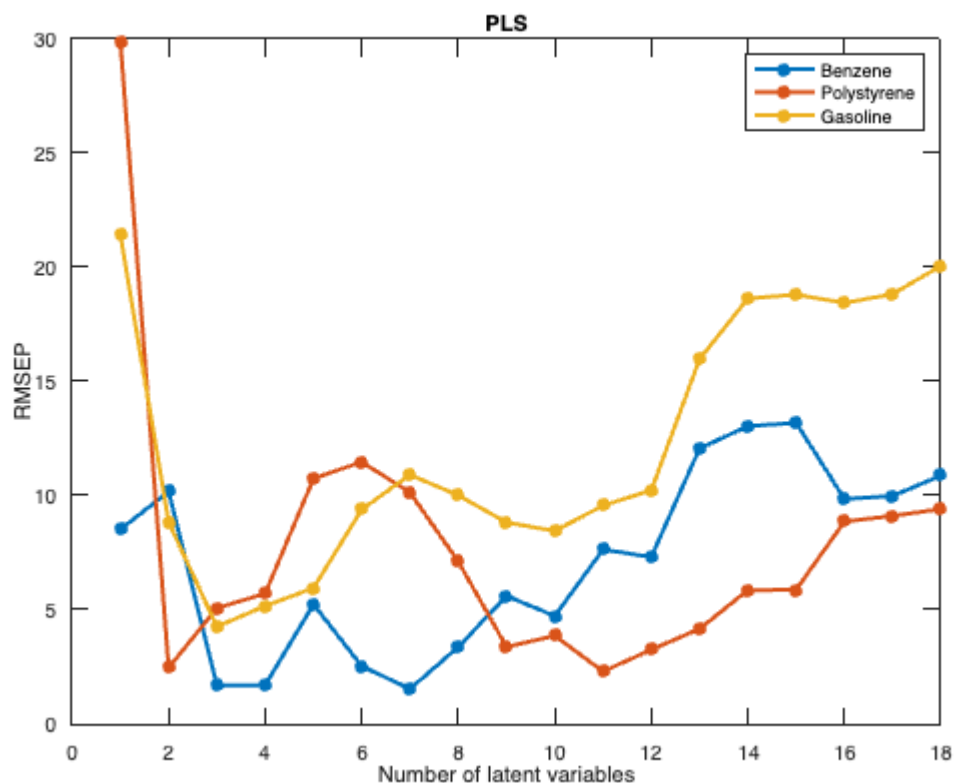
Name	Size	Bytes	Class	Attributes
A_train	20x1713	274080	double	
A_unknown	12x1713	164448	double	
C_train	20x3	480	double	
C_validation	12x3	288	double	
ConcentrationUnits	1x4	8	char	
ConstituentNames	1x3	364	cell	
WavenumberLabel	1x20	40	char	

Wavenumbers	1x1713	13704	double
ans	1x1	8	double

Optimal number of latent variables for PLS with mean centering

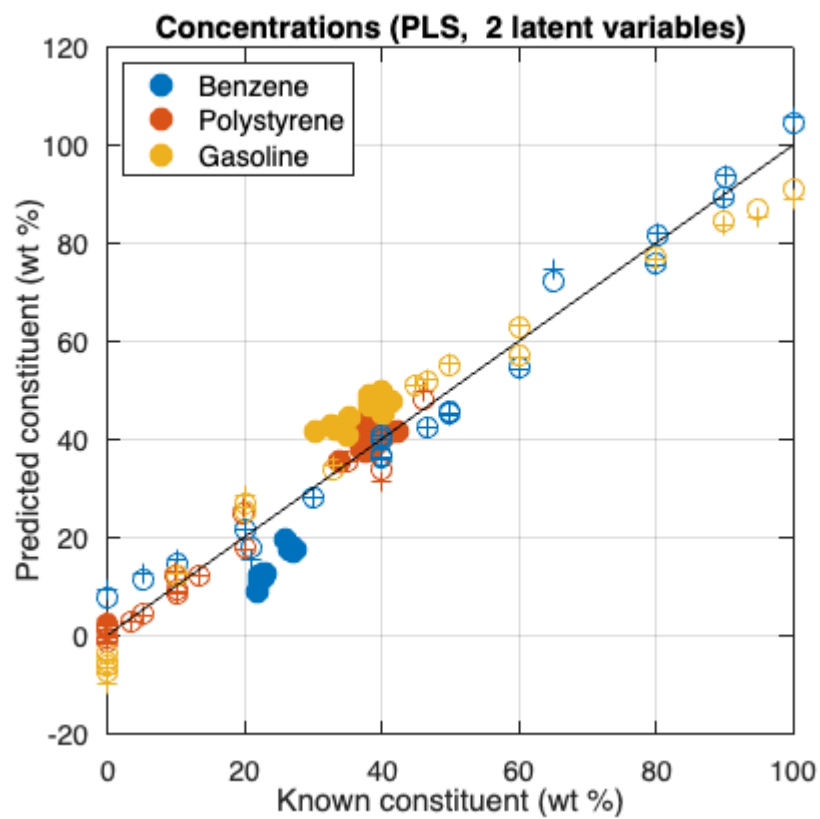
Compute PLS with mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;  
meanCentered = true;  
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);  
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)  
xlabel('Number of latent variables')  
ylabel('RMSEP')  
title('PLS')  
legend(ConstituentNames{:})
```



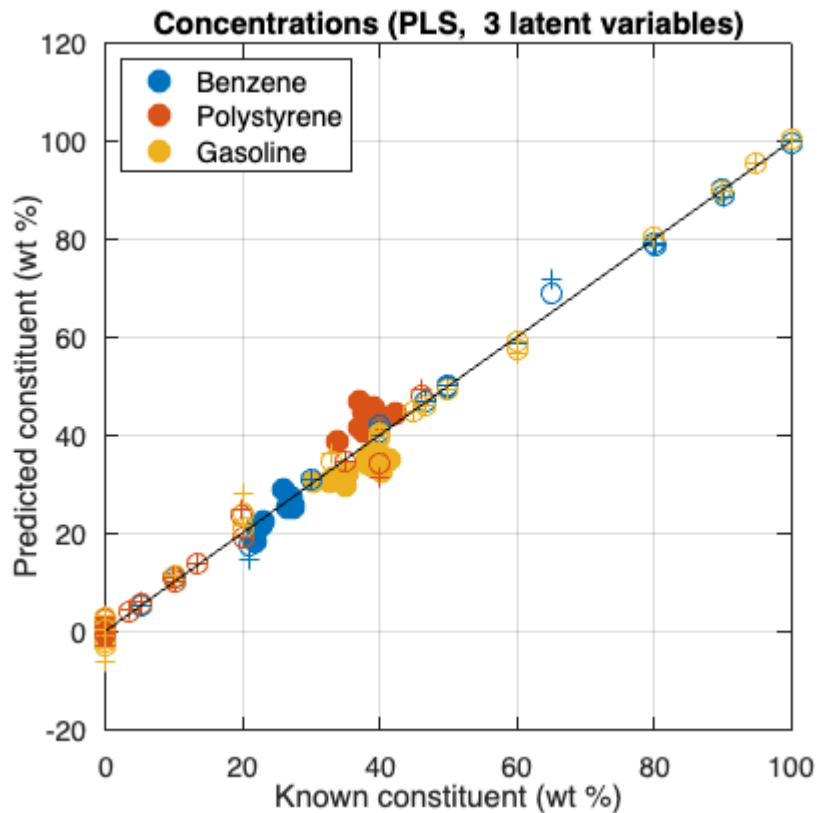
For mean-centered data, it looks like the knee in the curve for polystyrene is 2 latent variables, and 3 for benzene and gasoline. Plot them to see what they look like.

```
nLatentVariables = [2,3];  
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 2 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1479	2.296	5.5014
RMSECV	5.0229	2.924	6.5258
RMSEP	10.164	2.4566	8.8266



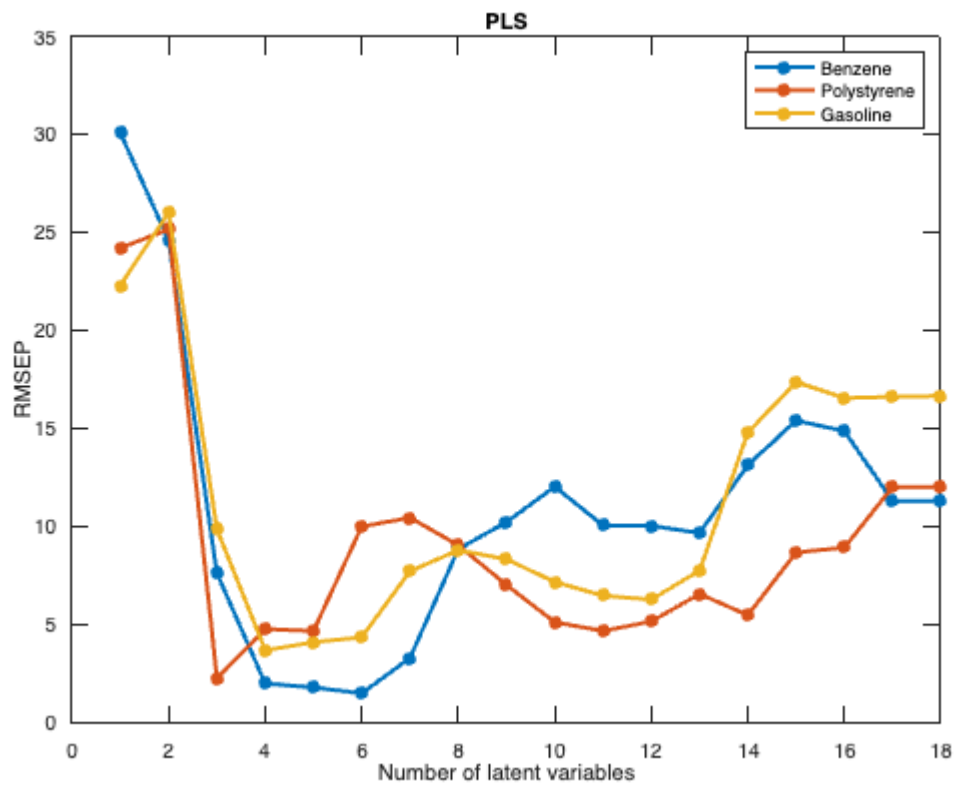
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.3968	1.8465	1.5789
RMSECV	2.2406	2.6176	2.7657
RMSEP	1.6799	5.0647	4.2528

Optimal number of latent variables for PLS without mean centering

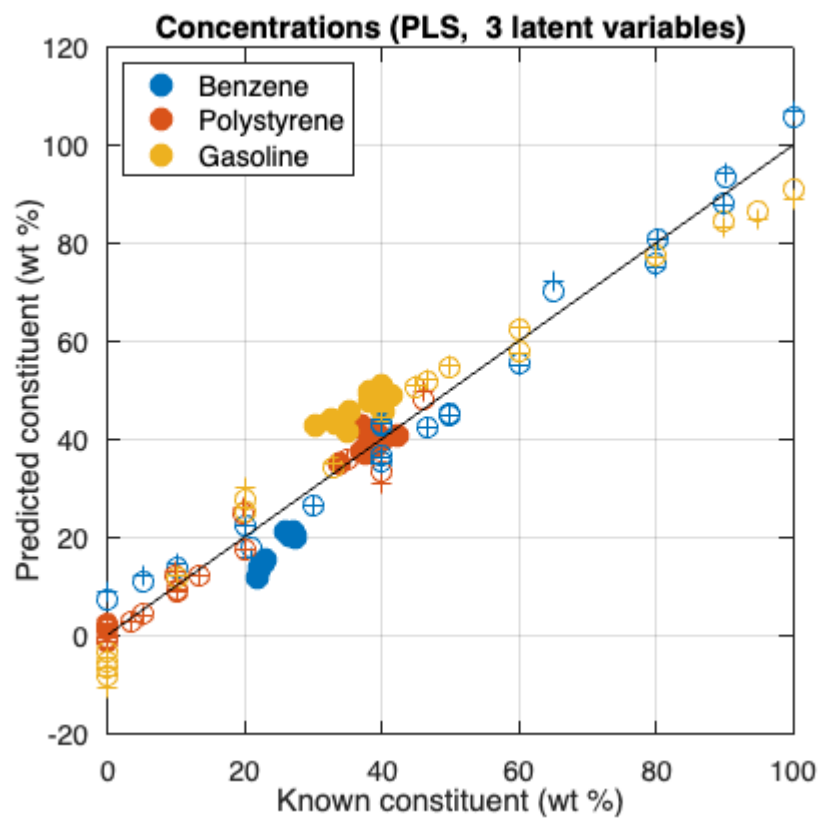
Compute PLS without mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = false;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



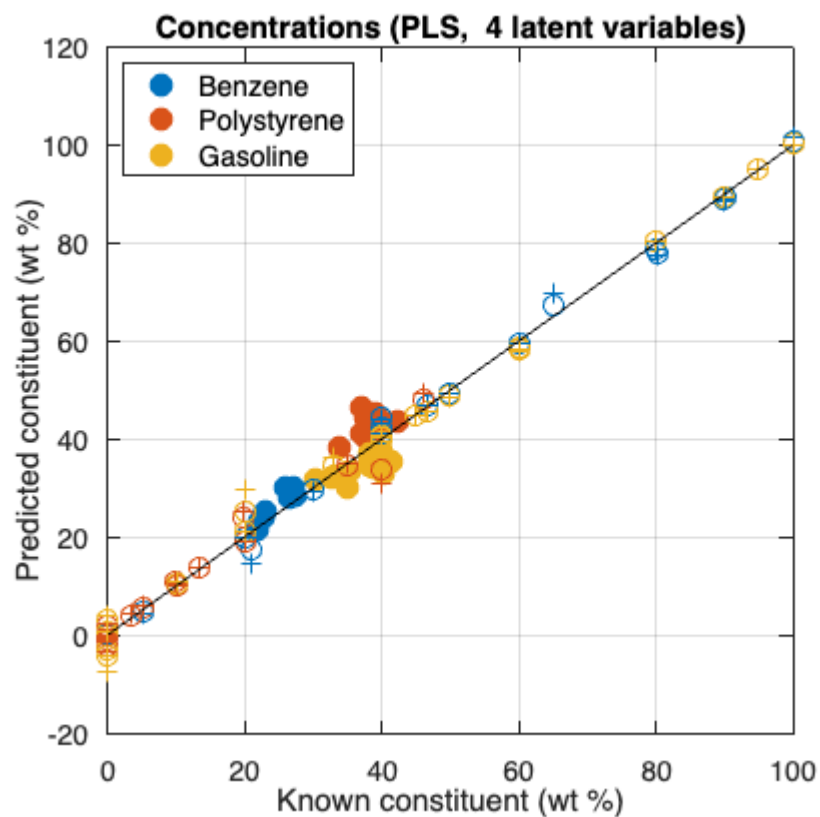
Without mean centering, it looks like the knee in the curve for polystyrene is 3 latent variables, 4 for gasoline, and 6 for benzene. Plot them to see what they look like.

```
nLatentVariables = [3 4 6];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



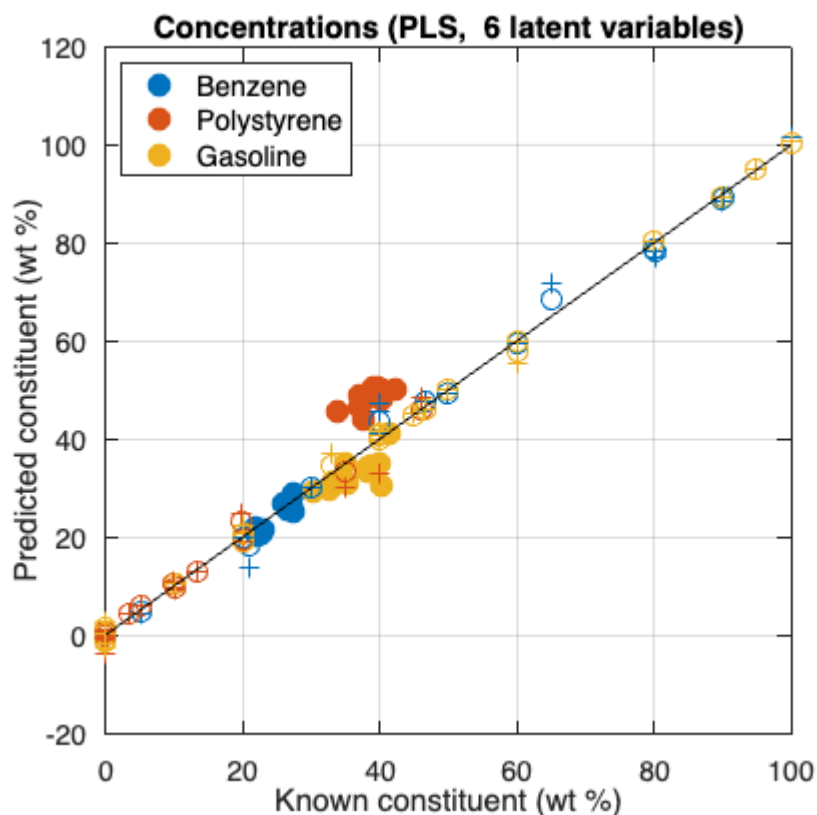
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1853	2.3592	5.6109
RMSECV	5.0232	2.9897	6.6976
RMSEP	7.5851	2.2404	9.8369



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 4 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.6636	1.921	1.9509
RMSECV	2.3112	2.6884	3.2095
RMSEP	1.9599	4.7379	3.6527



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 6 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.4134	0.99256	0.91242
RMSECV	3.1544	2.5526	1.7502
RMSEP	1.4567	9.9656	4.3211

Supresss editor warnings in this file.

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